Introduction To Quantum Mechanics

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Contents

Acknowledgement

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1 The Wave Function

What we are looking for is the **wave function $\boldsymbol{\Psi}$**.

Law 1.1 (Schrodinger Equation)**.**

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V\Psi.$$

For simplicity, we always rewrite it as:

$$i\hbar\partial_t\Psi=-\frac{\hbar^2}{2m}\partial_x^2\Psi+V\Psi.$$

Born's statistical interpretation:

$$\int_a^b|\Psi(x,t)|^2\,\mathrm{d}x=\text{probability of finding the particle between } a \text{ and } b \text{ at time } t.$$

Law 1.2 (Normalization)**.**

$$\int_{-\infty}^{\infty}|\Psi(x,t)|^2\,\mathrm{d}x=1.$$

Proposition 1.1. The wave function will always stay NORMALIZED.

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_{-\infty}^{\infty}|\Psi(x,t)|^2\,\mathrm{d}x=0.$$

Proof. By Schrodinger EQ.,

$$\text{LHS}=\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)\Big|_{-\infty}^{+\infty}.$$

□

Definition 1.1.

$$\langle x\rangle \overset{def}{=\!=} \int_{-\infty}^{\infty}x|\Psi|^2\,\mathrm{d}x$$

and

$$\langle p\rangle \overset{def}{=\!=} m\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t}.$$

Theorem 1.1.

$$\langle x\rangle=\int\Psi^*(x)\Psi\,\mathrm{d}x$$

and

$$\langle p\rangle=\int\Psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi\,\mathrm{d}x.$$

Remark 1.1 (Operator)**.** We say that the operator x represents position, and the operator $-i\hbar\,\partial/\partial x$ represents momentum. Also,

$$\langle Q(x,p)\rangle = \int_{-\infty}^{\infty} \Psi^* \left[Q(x, -i\hbar\frac{\partial}{\partial x}) \right] \Psi \,\mathrm{d}x.$$

Property 1.1. Operators do **NOT**, in general, commute. For example, $\hat{x}\hat{p} \neq \hat{p}\hat{x}$, i.e.,

$$\exists \text{ a function } f, \text{ s.t. } (\hat{x}\hat{p})f \neq (\hat{p}\hat{x})f.$$

Theorem 1.2 (de Broglie formula)**.** The wave length is related to the momentum of the particle:

$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda}.$$

Theorem 1.3 (Heisenberg's uncertainty principle)**.**

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}.$$

2 Time-independent Schrodinger Equation

2.1 Stationary states

We look for solutions that are simple products,

$$\Psi(x,t) = \psi(x)\varphi(t).$$

Theorem 2.1. By the method of separation of variables,

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V\psi = E\psi$$

and

$$\varphi(t) = e^{-iEt/\hbar}.$$

The first is called the **time-independent Schrodinger equation**.

Definition 2.1 (Hamiltonian)**.** In classical mechanics, the total energy (kinetic plus potential) is called Hamiltonian:

$$H(x,p) = \frac{p^2}{2m} + V(x).$$

Now we introduce **Hamiltonian operator**:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x).$$

Thus the time-independent Schrodinger EQ. can be written

$$\hat{H}\psi = E\psi$$

which is **IMPORTANT**.

Remark 2.1. Intriguingly and intuitively,

$$\langle H \rangle = E.$$

Also, if the equation yields an infinite collection of solutions $(\psi_1(x), \psi_2(x), \cdots)$, each with its associated value of the separation constant $(E1, E2, \cdots)$; thus the wave function is:

$$\Psi(x,t) = \sum_{n=1}^{+\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}.$$

Particularly,

$$E_n \geq 0 \text{ for all } n$$

2.2 The infinite square well

Suppose

$$V(x) = \begin{cases} 0 & \text{if } 0 \leq x \leq a \\ \infty & \text{otherwise} \end{cases}.$$

Theorem 2.2. Inside the well, we have

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2}$$

and

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right).$$

Property 2.1. $\psi_n(x)$ has some interesting and important porperties:

1. They are alternately even and odd, with the respect to the center of the well.
2. They are mutually orthogonal (i.e., $\int \psi_m(x)^* \psi_n(x)\, \mathrm{d}x = \delta_{mn}$) where δ_{mn} is **Kronecker delta**:

$$\delta_{mn} = \begin{cases} 0, & \text{if } m \neq n \\ 1, & \text{if } m = n \end{cases}.$$

3. They are complete by Dirichlet's theorem.

2.3 The harmonic oscillator

Let

$$V(x) = \frac{1}{2} m \omega^2 x^2.$$

Here I will introduce 2 entirely different approaches to this problem. The first is a diabolically clever algebraic technique and the second is a straitforward "brute force" solution.

2.3.1 Algebraic method

To begin with, let's rewrite the EQ. in a more suggestive form:

$$\frac{1}{2m}\left[\left(-i\hbar\frac{\mathrm{d}}{\mathrm{d}x}\right)^2 + (m\omega x)^2\right]\psi = E\psi.$$

The idea is to factor the term in square brackets:

$$u^2 + v^2 = (u - iv)(u + iv).$$

Definition 2.2 (Ladder operator).

$$\hat{a}_{\pm} = \frac{1}{\sqrt{2\hbar m\omega}}(\mp i\hat{p} + m\omega x).$$

Definition 2.3 (Commutator). The commutator of operators $\hat{A}$ and $\hat{B}$ is

$$\left[\hat{A}, \hat{B}\right] \xlongequal{def} \hat{A}\hat{B} - \hat{B}\hat{A}.$$

Property 2.2.

$$[\hat{a}_-, \hat{a}_+] = 1.$$

Theorem 2.3. If ψ satisfies the Schrodinger's EQ. with energy E, then $\hat{a}_+\psi$ satisfies the Schrodinger's EQ. with energy $E + \hbar\omega$:

$$\hat{H}\psi = E\psi \Longrightarrow \hat{H}(\hat{a}_+\psi) = (E + \hbar\omega)(\hat{a}_+\psi).$$

Similarly,

$$\hat{H}\psi = E\psi \Longrightarrow \hat{H}(\hat{a}_-\psi) = (E - \hbar\omega)(\hat{a}_-\psi).$$

Proof.

$$\hat{H} = a_+a_- + \frac{1}{2}\hbar\omega.$$

□

Here, then, is a wonderful machine for generating new solutions——if we could just find one solution. Thus, we call $\hat{a}_+$ raising operator and $\hat{a}_-$ lowering operator.
But what if I apply the lowering operator **repeatly**? We will reach a state with energy less than zero. By 2.1, there is **NO** guarantee that it will be normalized.

Proposition 2.1. Thus, there occurs a "lowest rung" ψ_0 such that

$$\hat{a}_-\psi_0 = 0.$$

Theorem 2.4.

$$\psi_0(x) = A_0 e^{-m\omega/2\hbar\, x^2}$$

and

$$E_0 = \frac{1}{2}\hbar\omega.$$

Thus we could get

$$\psi_n(x) = A_n (a_+)^n e^{-m\omega/2\hbar\, x^2}, \text{ with } E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

where A_n are used for normalization.

Theorem 2.5. ψ_n and ψ_{n+1} should satisfy:

$$\begin{cases} a_+\psi_n = i\sqrt{(n+1)\hbar\omega} \\ a_-\psi_n = -i\sqrt{n\hbar\omega}\psi_{n-1} \end{cases}.$$

Proof.

$$\int_{-\infty}^{\infty} |a_+\psi_n|^2 \,\mathrm{d}x = (n+1)\hbar\omega$$

and

$$\int_{-\infty}^{\infty} |a_-\psi_n|^2 \,\mathrm{d}x = n\hbar\omega.$$

□

Ultimately,

$$A_n = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{(-i)^n}{\sqrt{n!(\hbar\omega)^n}}.$$

2.3.2 Analytic method

Things look a little cleaner if we introduce the dimensionless variables

$$\xi = \sqrt{\frac{m\omega}{\hbar}}x \text{ and } K = \frac{2E}{\hbar\omega}.$$

In terms of ξ and K, the Schrodinger equation reads

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}\xi^2} = (\xi^2 - K)\psi.$$

To begin with, consider that at very large ξ, ξ^2 completely dominates over the constant K, so in this regime $\mathrm{d}^2\psi/\mathrm{d}\xi^2 = \xi^2\psi$, which means that $\psi \Longrightarrow Ae^{\xi^2/2} + Be^{-\xi^2/2}$. Thus we let $\psi = h(\xi)e^{-\xi^2/2}$. Plugging ψ into Schordinger EQ., we have

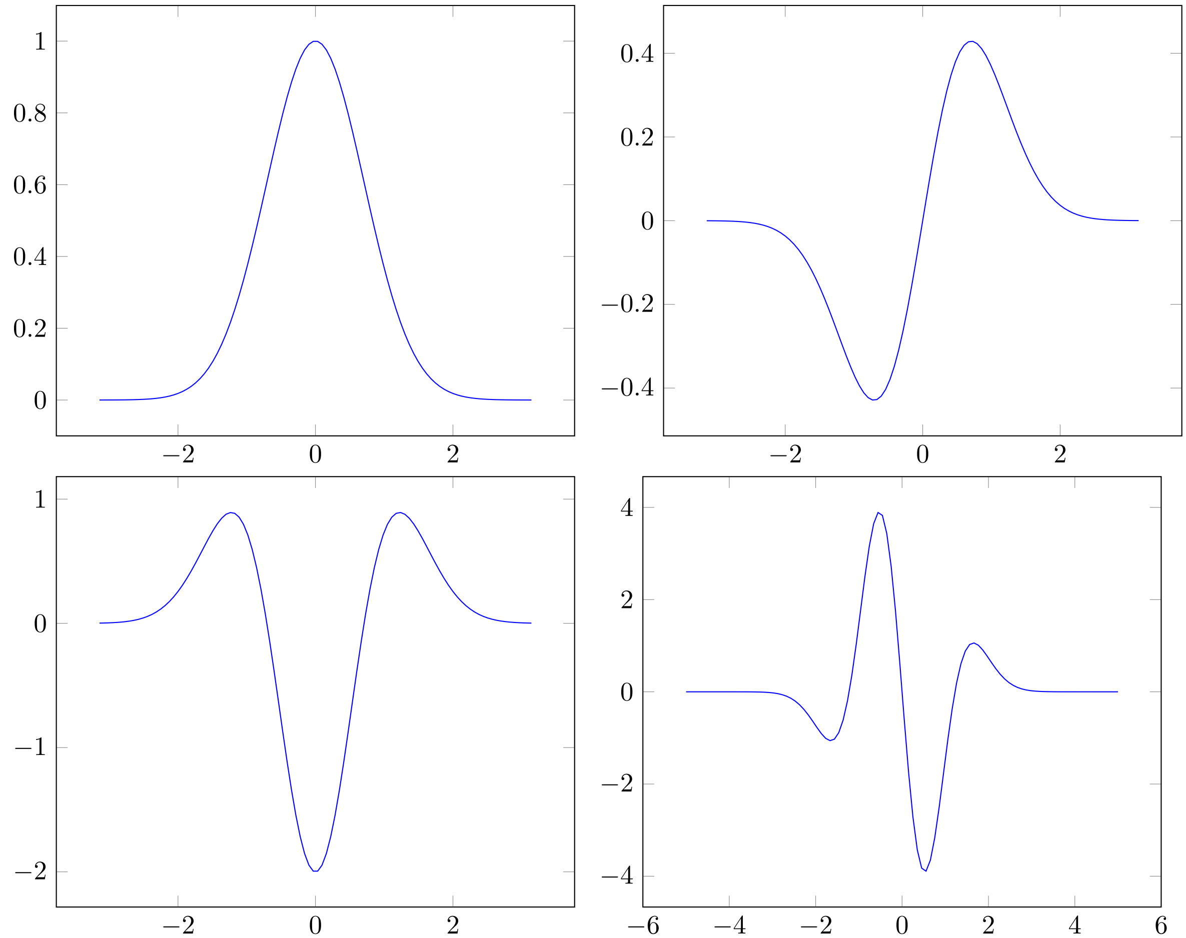
$$h(\xi) = \sum_{n=0}^{\infty} a_n \xi^n \text{ and } a_{n+2} = \frac{2n+1-K}{(n+1)(n+2)}.$$

For physically acceptable solutions (normalizable solutions), then, we must have $K = 2n+1$. Finally,

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\xi^2/2}$$

where H_n is the **Hermite polynomials**.

The first four stationary states of the harmonic oscillator are as follows.



2.4 The Free Particle

We turn next to what should have been the simplest case of all: the free particle. The time Schrodinger Eq. reads:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = E\psi.$$

Let $k \equiv \sqrt{2mE/\hbar}$, we have

$$\Psi_k(x,t) = Ae^{i(kx - \hbar k^2 t/2m)}.$$

Remark 2.2. The speed of these waves is:

$$v_{\text{quantum}} = \sqrt{E/2m} = 0.5 v_{\text{classical}}$$

And

$$\int_{-\infty}^{\infty} \Psi_k^*(x,t)\Psi_k(x,t)\,\mathrm{d}x = +\infty,$$

which means that a free particle cannot exist in a stationart state.

Theorem 2.6. The general solution to the time-independent Schrodinger EQ. is still a linear combination of separable solutions:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \hbar k^2 t/2m)} \, \mathrm{d}k.$$

Now this wave function can be normalized for appropriated $\phi(k)$. We call it a **wave packet**.

Definition 2.4 (phase velocity and group velocity)**.** For the wave function:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{i(kx - \omega t)} \, \mathrm{d}k.$$

We define:

$$v_{\text{phase}} = \frac{\omega}{k}, \ v_{\text{group}} = \frac{\mathrm{d}\omega}{\mathrm{d}k}.$$

3 Formalism

3.1 Gerneralized Statistical Interpretation

First we assume the spectrum of the wave funtion is discrete, we have

$$\langle Q \rangle = \sum_{n'} \sum_{n} c_{n'}^* c_n q_n \langle f_{n'} | f_n \rangle = \sum_n |c_n|^2 q_n$$

where q_n is the eigenvalue of operator $\hat{Q}$ and $\Psi(x,t) = \sum_n c_n(t) f_n(x)$. What about momentum?

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \Psi(x,t) \, \mathrm{d}x$$

and

$$\Phi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-ipx/\hbar} \Phi(p,t) \, \mathrm{d}p.$$

3.2 Uncertainty Principle

Theorem 3.1 (generalized uncertainty principle)**.**

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \left\langle \left[\hat{A}, \hat{B} \right] \right\rangle \right)^2.$$

How to interpret Δt?

Definition 3.1.

$$\Delta t \equiv \frac{\sigma_Q}{|\mathrm{d} \langle Q \rangle / \mathrm{d}t|},$$

where

$$\frac{\mathrm{d} \langle Q \rangle}{\mathrm{d}t} = \frac{i}{\hbar} \left\langle \left[\hat{H}, \hat{Q} \right] \right\rangle + \left\langle \frac{\partial \hat{Q}}{\partial t} \right\rangle.$$

I recommend you to learn **Hilbert space** and **Dirac notation**.